

Rhodopsin

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<http://web.me.com/whitby/Octahedron/Welcome.html>

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Rhdopsn.pdf

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Bacteriorhodopsin

Description

Bacteriorhodopsin is described in the literature as a single peptide having seven closely packed alpha helices. The helical axes are parallel. An arrangement of parallel helices is shown near the end of the chapter CYCLIC in *Octahedron, 1st Ed.* page 380. The features used to produce the cyclic peptide are used here to produce a structure similar to that of bacteriorhodopsin.

Sequence

There are 348 residues in a bacteriorhodopsin sequence.¹ This provides 116 triplets. Four residues are required for each of the six 32chain links between adjoining helices which accounts for twenty-four residues. Seven helices of fifteen turns of three residues each accounts for 315 residues. The helices and the links together use 339 residues leaving nine unallotted residues.

Helical length

The axial length of an alpha helix is equal to the axial width of the first residue plus the number of additional residues it contains times the axial rise per residue. The axial width of the first residue is three He-octa facial diameters. The rise per additional residue is one facial diameter. The fifteen turn helix has three residues per turn for forty-five residues total. The overall length is forty-seven facial diameters—three for the first residue plus forty-four for the additional residues. Using the He-octa edge length of 1.1825A derived from Pauling and Corey and letting L denote the overall

length of the alpha helix

$$L = 47 \times 1.1825A \times \sqrt{\frac{2}{3}} = 45.37A$$

This matches the 45A purple membrane width of the *Halobacterium halobium*.²

Structure

The three following figures show how the main chain portions of the amino acids produce the structure of bacteriorhodopsin. In each of the figures,, the helical axes are perpendicular to the projection plane which is parallel to the membrane surface.

The first figure shows that the structure is produced by main chain units which have only six orientations—three to produce an ascending helix and three to produce a descending helix. Residues having the same helical orientations join as 32chains to link the helices. At each terminus of the 32chain link, the join between the helix and the 32chain continues the 32chain. The structure in the first figure is the most compact arrangement of this type which is possible—there are just two residues between the helices. While the final assembly here shows six helices, the structural motif can produce any number of parallel alpha helices linked in a single chain.

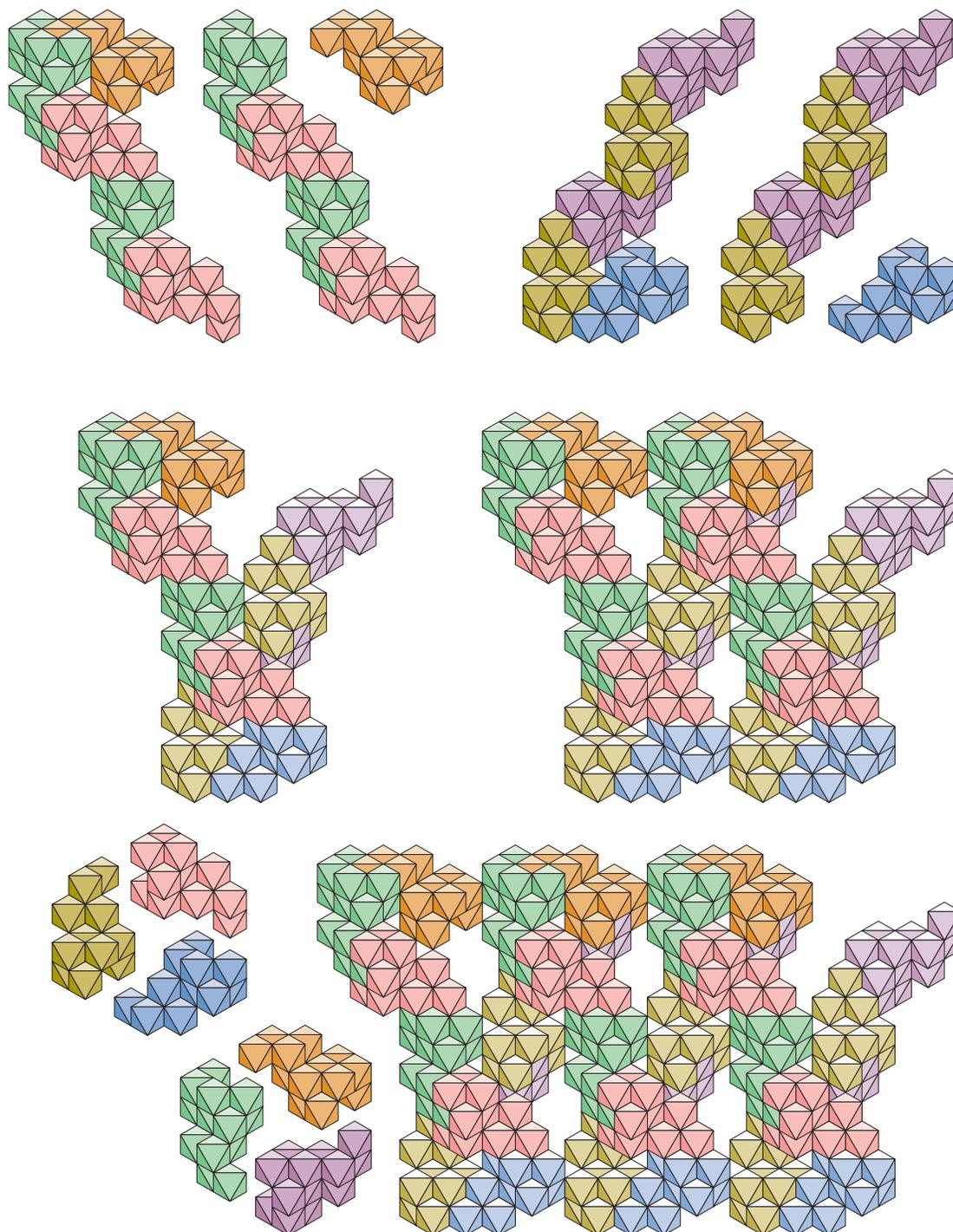
The second figure extends the 32chains by two residues and shows them joined in the same way as those in the most compact assembly.

The third figure extends the helices and shows how the side chains are disposed.

1. Lauren E. Ball *et al*, Mass spectrometric analysis of integral membrane proteins: Application to complete mapping of bacteriorhodopsin and rhodopsin, *Protein Science* (1998), 7:758-764, Cambridge U. Press.

2. Lubert Stryer *Biochemistry*, 2d Ed., W. H. Freeman, 1981, pp. 227-228.

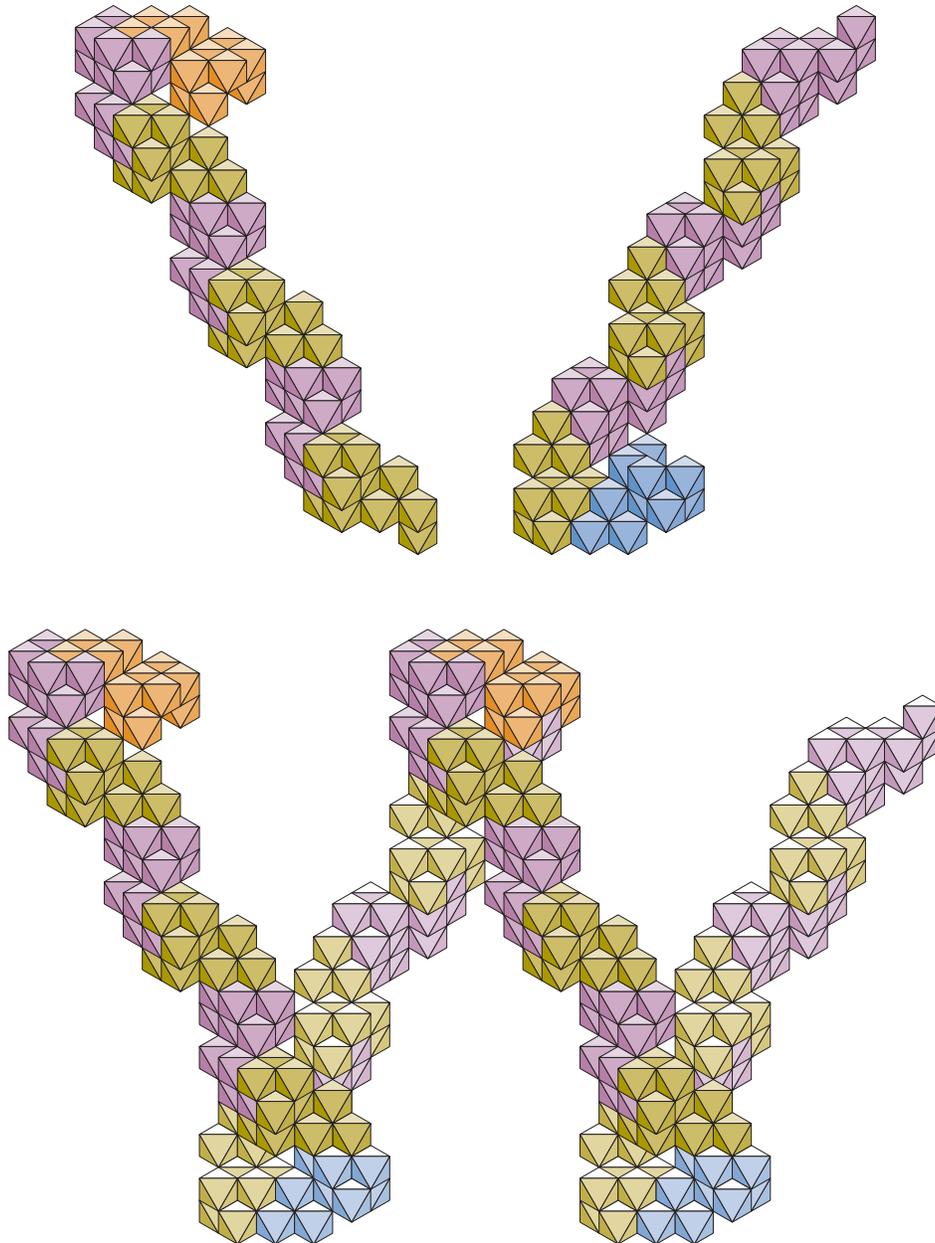
Compact chain of parallel helices



Most compact chain of parallel-axised alpha helices linked by 32chains.

The two groups of three main chain units each in the lower left hand corner of the figure are used to produce the two subassemblies at the top of the figure. The subassemblies join so as to complete an alpha helical turn. The subassemblies which are paired on the left side of the middle row are combined with a like pair to produce the assembly to its right. A third pair has been added to produce the assembly on the bottom right. The three helices at the top are ccw ascending and the three at the bottom are cw descending.

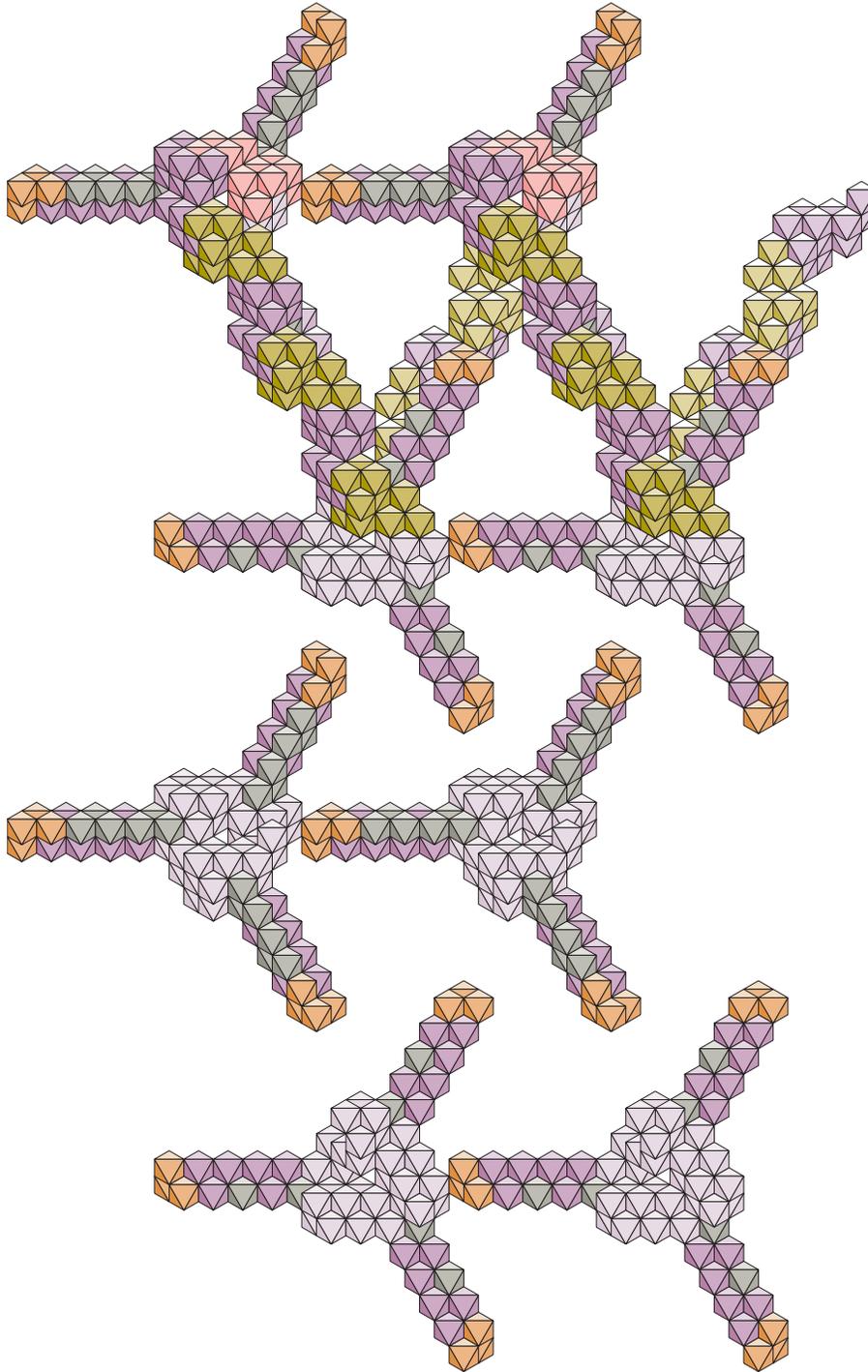
Parallel helices with extended links



Chain of alpha helices linked with extended 32chains.

The 32chains of the two subassemblies of the previous figure have been extended by the insertion of a pair of residues to produce the subassemblies at the top of this figure. The join between the extended subassemblies is identical to that between the previous subassemblies. Four of the extended subassemblies have been used to produce the chain at the bottom of the figure.

Parallel helices with side chains



Extending the helices of the peptide chain.

Each of the four helices of the previous figure has been extended by a single turn composed of three lysine residues to produce the peptide chain at the top of this figure. The added turns are shown separately at the bottom of the figure in the same relationship that they have within the chain. The spacing between the helices is the same as occurs in bacteriorhodopsin.

Bovine rhodopsin p22121 crystal

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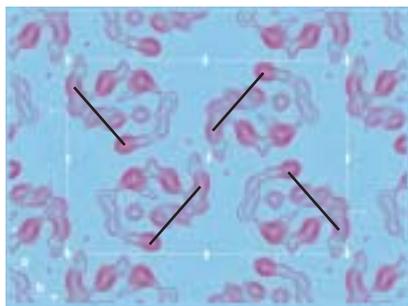
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References

1. Krebs, A., Villa, C., Edwards, P.C., & Schertler, G.F. (1998). Characterisation of an improved two-dimensional p22121 crystal from bovine rhodopsin. *J Mol Biol*, 282 (5), 991-1003.
2. Octahedron1stEd.pdf
3. rhdopsn.pdf
4. 32chain.pdf
5. <http://www2.mrc-lmb.cam.ac.uk/groups/GS/Poster/posterimages/fig4.gif>

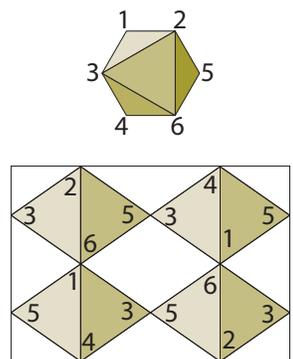
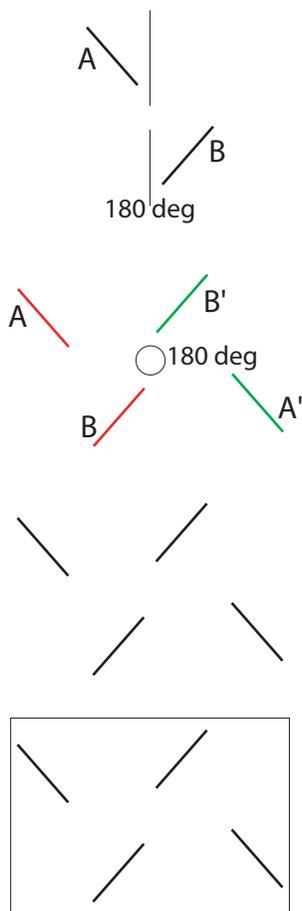
Introduction

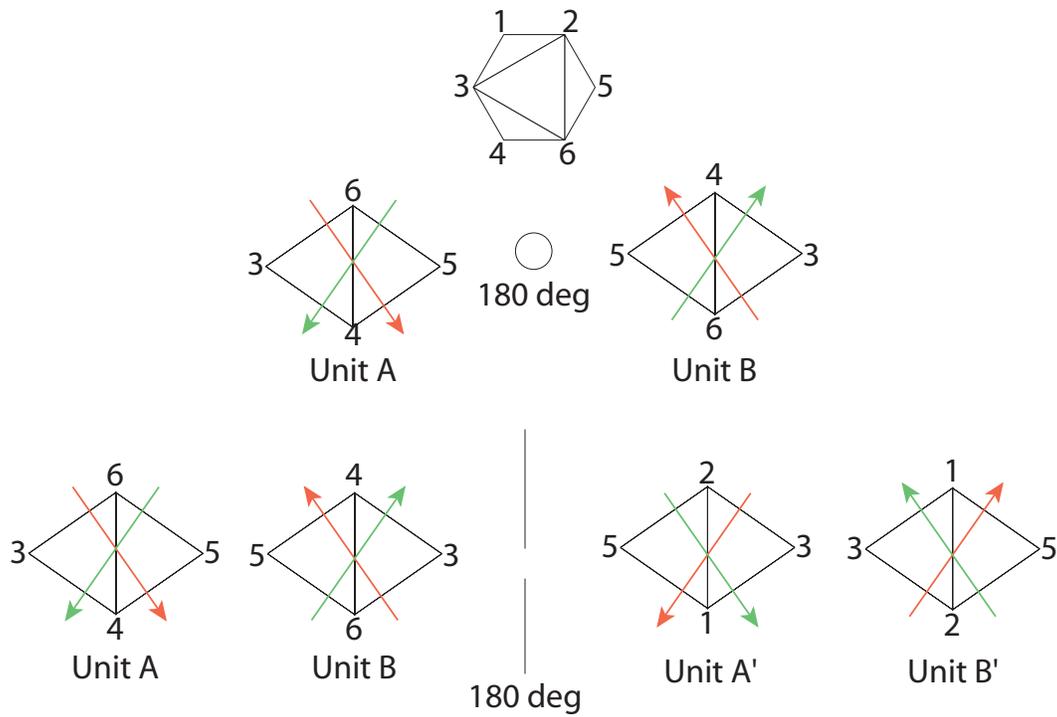
The projection density map of the p22121 crystal of bovine rhodopsin [Ref. 1] provides an orientation for the identical octahedra which make up the atoms of the protein molecules.



Bovine rhodopsin crystal

The <projection density map of bovine rhodopsin p22121 crystals to 5 Å> [Refs. 1 & 5] is shown with permission at the top left of the figure. Lines have been used to connect the same pair of features on each of the four molecular projections of the delineated unit cell. The relationships between the orientations of the molecules are shown in the two rotational diagrams just below the density map. At the bottom left, the group of lines is shown first separately and then within the rectangular confines of the unit cell. The ratio of the length to the width of this rectangle is approximately $\sqrt{2}$. This ratio is the same as the ratio of the vertexial diameter of an octahedron to its edgial diameter. The rotational relationships between the molecules together with the diameter ratio of the unit cell suggests that each of the identical octahedra which compose the atoms of the molecules is oriented as shown in the four edgial views enclosed within the unit cell rectangle at bottom right. A facial view of a regular octahedron with its vertexes labeled for reference is shown just above it. Each edgial view represents the orientation of one of the four molecules. The one on the upper left is molecule *A*, below it is molecule *B*, and the two to the right are molecules *B'* and *A'*. Each of the views here is perpendicular to the plane of the crystal.





Bovine rhodopsin crystal-alpha-helical axes

The figure shows the relationships between the alpha helical axes of identical units whose relative orientations are identical to the molecules of the bovine rhodopsin crystal. The view here is parallel to the crystalline plane and at right angles to that of the previous figure. The axes of those alpha helices which are not parallel to the crystal plane are represented by the green and red arrows. Each of these axes makes an angle of $\text{atan}\sqrt{2}$ with the plane of the crystal.

